May 26, 1971

FRA-TM-13

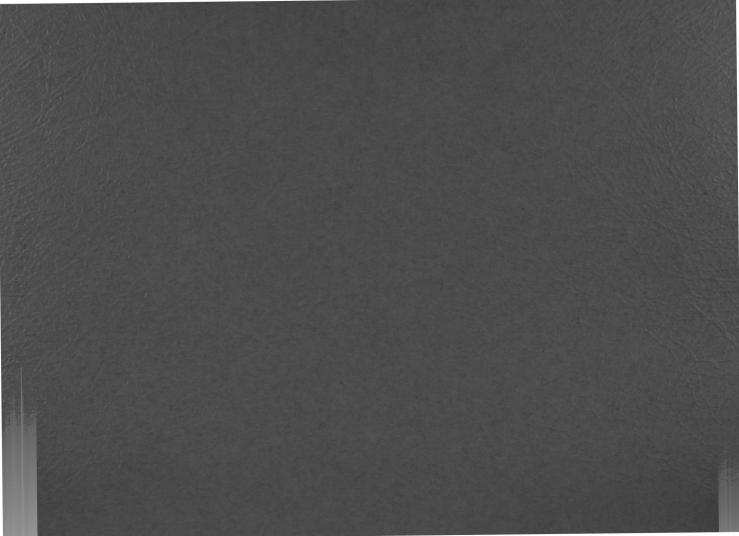
EVALUATION OF SPACE-ENERGY FACTORIZATION FOR TWO-DIMENSIONAL LMFBR DIFFUSION THEORY PROBLEMS

Weston M. Stacey, Jr.

Argonne National Laboratory Applied Physics Division 9700 South Cass Avenue Argonne, Illinois 60439

FRA TECHNICAL MEMORANDUM NO. 13

Results reported in the FRA-TM series of memoranda frequently are preliminary and subject to revision. Consequently they should not be quoted or referenced without the author's permission.



Evaluation of Space-Energy Factorization for Two-Dimensional LMFBR Diffusion Theory Problems

Weston M. Stacey, Jr.

Applied Physics Division, Argonne National Laboratory
Argonne, Illinois 60439

Use of a space-energy factorization (SEF) scheme to obtain approximate solutions to the energy-dependent neutron diffusion equation was suggested in Ref. 1, where the method was successfully applied to one-dimensional/24-group LMFBR models. Initial applications of the method to two-dimensional/24-group and one-dimensional/165-group LMFBR models were reported in Ref. 2. The purpose of this note is to report the results of subsequent numerical studies undertaken to evaluate the efficacy of the method for two-dimensional/24-group LMFBR models.

SEF has been incorporated into the inner iteration to obtain an approximate solution to

$$H(r,E)\phi(r,E) = \int_{E}^{\infty} dE' K(r,E' \rightarrow E) \phi(r,E') + S(r,E)$$
 (1)

by factoring the flux within each of several shape function intervals $\mathbf{E_g} \le \mathbf{E} \le \mathbf{E_{g+1}} \text{ in the form}$

$$\phi(\mathbf{r}, \mathbf{E}) \sim \mathbf{a}(\mathbf{E})\psi_{\mathbf{g}}(\mathbf{r}) , \qquad \mathbf{E}_{\mathbf{g}} \leq \mathbf{E} \leq \mathbf{E}_{\mathbf{g}+1} .$$
 (2)

Substituting relation (2) into Eq. (1) and integrating over the interval $E_g \leq E \leq E_{g+1} \mbox{ yields equations for the shape functions, } \psi_g$

$$\begin{bmatrix} E_{g+1} \\ E_g \end{bmatrix} dE H(r,E)a(E) \psi_g(r) = \int_{E_{g'}}^{E_{g+1}} dE S(r,E)$$

$$+ \sum_{g' \leq g} \left[\int_{E_g}^{E_{g+1}} dE \int_{E_g}^{E_{g'+1}} dE' K(r,E' + E)a(E') \right] \psi_{g'}(r) ,$$

(3)

and the same substitution together with an integration over space yields an equation for the spectral function, a(E),

$$\left[\int d\mathbf{r} \ H(\mathbf{r}, E) \psi_{\mathbf{g}}(\mathbf{r}) \right] a(E) = \int d\mathbf{r} \ S(\mathbf{r}, E)$$

$$+ \sum_{\mathbf{g}' \leq \mathbf{g}} \int_{E_{\mathbf{g}'}}^{E_{\mathbf{g}'}+1} dE' \left[\int d\mathbf{r} \ K(\mathbf{r}, E' + E) \psi_{\mathbf{g}'}(\mathbf{r}) \right] a(E') \ . \tag{4}$$

In a typical calculation reported in this note, employing six shape-function intervals, Eq. (4) would be solved on a 24-group basis for a(E). The interval $E_g \leq E \leq E_{g+1}$ would contain 4 of the 24 groups, thus Eqs. (3) would be solved on a 6 broad-group basis.

On each inner iteration, ψ_1 from the previous inner iteration is used to evaluate the spatial integrals in Eq. (4). Then a(E), $E_1 \leq E \leq E_2$, is obtained by solving Eq. (4), and used to evaluate the energy integrals over this interval in Eqs. (3). Then Eq. (3) is solved for ψ_1 . This

Substituting relation (2) into Eq. (1) and integrating over the interval Eq. (1) for the shape functions, a

(63)

and the same substitution together with an integration over space youlds an equation for the epochval function, a(E).

In a typical calculation reported in this note, enricying six shape-function intervals, Eq. (4) would be solved on a 24-group basis for a(2). The inverval $E_g \le E \le E_{g+1}$ would contain 4 of the 24 groups, thus Eqs. (3) would be solved on a 5 broad-group basis.

On each inner iteration, v, from the previous irrer iteration is used to evaluate the sparial integrals in Eq. (4). Then a(E), E, _ E < F2, is obtained by solving Eq. (4), and used to evaluate the energy integrals over this interval in Eqs. (3). Then Eq. (3) is solved for eq. This

value of ψ_1 , and ψ_2 from the previous inner iteration, are used to evaluate the spatial integrals in Eq. (4), which is solved for a(E), $E_2 \leq E \leq E_3$. This value of a(E) is used to evaluate the energy integrals over this interval in Eqs. (3), which are then solved for ψ_2 . This process is repeated for all shape function intervals.

The solution of Eqs. (3), which are formally identical to the multigroup equations, is accomplished iteratively with an ADI-B² method similar to that of Ref. 3. Equation (4), which is identical to the fundamental mode slowing-down equation, is solved directly.

Power iteration, with two-term Chebyschev extrapolation, was employed for the outer iterations. One inner iteration per outer iteration was used (i.e. the SEF procedure outlined above was used once each outer iteration, and a single sweep in each direction was used in solving Eq. (3) by the ADI-B² scheme). Numerical experiments revealed that the spectral function, a(E), did not change much from iteration to iteration after the first few iterations. Accordingly, the spectral function was recalculated each iteration for the first five iterations, and subsequently only recalculated every fifth outer iteration. For the direct 24-group solution the same iteration scheme was used (i.e. power iteration with two-term Chebyschev extrapolation on the outer), so that a meaningful evaluation of the computational savings associated with the SEF method could be made.

Numerical studies of the SEF method were performed on three reactor models typical of proposed LMFBRs. The geometric model is shown in Fig. 1 (for Model 3 the X-dimensions were 50, 40, 40, and 10 cm), and the compositions are given in Table I. Model 1 is very similar to models which have been used in preliminary design studies for LMFBRs. Model 2

cains of \$1, and \$2 from the provious inner iteration, are used to evaluate the epsilel integrals in Eq. (4), which is solved for a(E),

by S E S E, This value of all is used to evaluate the energy integrals over this interval in Eqs. (3), which are then solved for v. This process is to exact for all shape function intervals.

The solution of Eqs. (3), which are formally identical to the multigroup equations, is accomplished fragatively with an AM-R² merical plants
law to them of Def. 3. Equation (A), which is identical to the fundamental mode slowing-down equation, is solved directly.

Four iteration, with two-term Combustions warrespolation, was employed for the outer iterations. One innot iteration per outer iteration was used (i.e. the SEE procedure outlined above was used once each cutter iteration, and a single meson in each direction vas used in colving Eq. (3) by the ADI-8² scheme). Numerical experiments revealed that the appeared function, a(E), aid not charge much from instation to iteration after the first the first time first time first time first time first time first time in white each iteration for the first time iterations, and when quently only recalculated every fifth outer iteration. For the direct with two term content on the case was used (i.e. power trustion with two term Content and a restriction on the case with the computational eavings associated with the SEE method could be made.

Numerical studies of the Sil method were performed on three resotor a models typical of proposed LATENS. The geometric model is shown in Fig. 1 (for Model 3 the X-dimensions were 50, 00, 00, and 10 unl, and 10 objectivious are given in Table 1. Model I is very similar to models which have been used in trailminary design studies for LYTENS. Model 2

differs from Model 1 only in that the sodium has been completely voided from Core 2 and Axial Blanket 2, and represents a hypothetical accident condition. Model 3 was chosen to provide a more difficult test of the SEF method; the sodium content in the two core regions is significantly different and a significant amount of plutonium has been included in the blankets.

The objectives of these studies were to evaluate the accuracy and computational economy of the SEF method, particularly relative to the similar but simpler few-group approximations obtained by group collapsing, and to evaluate the efficacy of using the fission source from the SEF solution as an initial guess to accelerate the convergence of direct 24-group solutions. The few-group constants were obtained by collapsing over a critically buckled 24-group spectrum for the composition of Core 1.

Results shown in Table II indicate that the SEF method is significantly more accurate in the prediction of criticality than a few-group method which employs the same number of spatial-shape calculations. Callations with only two shape functions are significantly more accurate than two-group calculations in predicting the maximum power peaking, and the six-shape function calculation is somewhat superior to the six-group calculation in this respect. Regional power fractions are predicted better by the two-shape function calculation than by the two-group calculation, but there is little difference between the six-shape function and six-group predictions, as indicated in Tables III-V. Power distributions along the horizontal and vertical centerlines of Model 3 are shown in Figs. 2 and 3.

For Models 1 and 2 the few-group predictions of breeding ratios are somewhat better than the corresponding SEF predictions, due to compensating

differs from Model 1 only in that the sodium has been completely voided from Core 2 and Axial Slanker 2, and représents a hypothetical accident condition. Model 3 was chosen to provide a more difficult rest of the SET method; the sodium content in the tou core regions is significantly different and a significant encurt of plutonium has been included in the blankets.

The objectives of these studies were to evaluate the accuracy and computational economy of the SEE method, purticularly relative to the similar but simpler few-group approximations obtained by group collapsing, and to evaluate the efficacy of using the fishion source from the SEE solution as an initial guess to accelerate the convergence of direct 24-group solutions. The few-group constants were obtained by collapsing over a critically buckled 24-group spectrum for the composition of Core 1.

Results shown in Table II indicate that the SET method is significantly more accurate in the prediction of criticality than a few-group method which employs the same number of spatial-shape calculations. dallations with unly two shape functions are significantly more accurate than two-group calculations in predicting the maximum power peaking, and the six-snape function calculation is somewhat superior to the six-group calculation in this respect. Regional power fractions are predicted better by the two-shape function calculation than by the two-group calculation, but there is little difference between the six-shape functions and six-group predictions, as indicated in Tables III-V. Power distributions along the horizontal and vertical centerlines of Model 3 are shown in Figs. 2 and 3.

For Models 1 and 2 the fer-group predictions of breeding ratios are somewhat betwee them the corresponding SEF predictions, due to corporating

errors in the few-group calculations which predict too hard a spectrum and too much flux in the blankets. This trend is reversed for Model 3. These results are shown in Tables III-V.

The computation times and number of outer iterations associated with the various calculations are shown in Table VI. The two-shape function calculation is roughly a factor of 5 quicker than the direct solution, and the six-shape function solution, which is quite accurate, is roughly a factor of 3 quicker than the direct solution. Few group solution times are 20-30% less than the corresponding shape function solution times. The computation of the collapsing spectrum and the preparation of the few-group constants has not been included in the former, but this will not significantly alter the comparison.

Use of the fission source from the SEF calculation as a first guess in the direct 24-group solution significantly reduces (25-40%) both the number of iterations and the total computing time relative to what is required when the standard flat fission source is used as a first guess. In this respect, use of the two-shape function solution is more economical than use of the more accurate six-shape function solution. Use of the fission source from the few-group calculations may also reduce the computing time required for the 24-group calculation, but this point has not been investigated.

In summary, the SEF method provides an economical means for obtaining approximate solutions to two-dimensional LMFBR diffusion theory problems. These solutions are sufficiently accurate for many applications,
and generally superior to the results of comparable few-group calculations.

Moreover, use of the SEF solution to accelerate the direct solution can
significantly reduce the computational time for the latter. Thus, it

moves in the fee-group calculations which predict too hard a spectrum and too much flue in the bianceie. This trend is revorsed for 19491 3.

These results are shown in Tables III.V.

The computation times and makes of outer iterations associated with the various calculations are shown in Table VI. The two-steps function calculation is roughly a factor of 5 quicker than the direct solution.

and the six-shape function solution, which is quite solution to including a factor of 3 quicker than the direct solution. For group believes times are 16-30% less than the conversations and the presention of the computation of the conversation of the conversation.

Die of the first a function comes from the SHT reliablishing so a first great in the direct in-roug solution significantly reduces (25-103) both the maker of directions and the total compating time relative to what is required show the character flat literian source is used as a first great in this respect, use of the name accurate him-chape function solution. Use of the final source from the farther solution and the foreign solutions are point the compating time that for the lateral order of the point had not been investigated.

In supercy, the SET derivat per idea on economical rease for obtaining approximate solutions to the dissipations in 1888 diffusion tracey probless. These solutions are sufficiently accounts for many applications,
and promising a partier to the results of comparable lest-group culculations.

Moreover, use of the SET solution to accelerate the direct solution can
eligible. The SET solution to accelerate the direct solution can

seems appropriate to conclude that the capability of multidimensional diffusion theory codes designed to solve 20- to 30-group LMFBR problems could be substantially enhanced by providing for the SEF calculation. The necessary modifications should be minor, because Eqs. (3) can be solved by the same routines which solve the conventional multigroup equations and the solution of Eq. (4) is trivial. The strategy outlined above for the SEF method is consistent with the group-ordering stategy employed in many diffusion theory codes, so no major changes in data management should be necessary.

Direction Ties-Differencing Sethate with Coase Delicit Sethids for

seems appropriate to conclude that the capability of multidimensional diffusion theory codes designed to solve 20- to 30-group LETE problems could be substantially enhanced by providing for the SEF calculation. The recessary modifications should be minor, because Eqs. (3) can be solved by the same routines which solve the conventional multigroup equations and the solution of Eq. (4) is trivial. The strategy curlined above for the SEF method is consistent with the group-ordering stategy employed in many diffusion theory codes, so no major charges in data management should be processary.

REFERENCES

¹W. M. STACEY, JR., "Solution of the Neutron Diffusion Equations by Space-Energy Factorization," *Nucl. Sci. Eng.*, to be published; also FRA-TM-3, Argonne National Laboratory (1970).

²W. M. STACEY, JR., and H. HENRYSON, II, "Applications of Space-Energy Factorization to the Solution of Static Fast-Reactor Neutronics Problems," *Proc. Conf. New Developments in Reactor Mathematics and* Applications, Idaho Falls, March 1971, The American Nuclear Society to be published; also FRA-TM-11, Argonne National Laboratory (1971).

³L. A. HAGEMAN and J. B. YASINSKY, "Comparison of Alternating Direction Time-Differencing Methods with Other Implicit Methods for the Solution of the Neutron Group-Diffusion Equations," *Nucl. Sci. Eng.*, 38, 8 (1969).

HEREITAGES

¹W. M. STACEY, JR., "Solution of the Neutron Diffusion Equations by Space-Energy Factorization," Nucl. Sal. Naj., to be published; also FRA-IM-3, Argonne National Laboratory (1978).

²W. M. STACET. JR., and H. HENRYSON. II, "Applications of Space-Energy Factorization to the Solution of Static Last-Resourn Meuronica Problems," Proc. Conf. New Daveleyments in Reactor Mathematics and Applications, Idaho Palls, March 1871, The American Miclear Scolery to be published; also RRA-IN-II, Argemen National Laboratory (1871).

*I. A. HARTMAN and J. B. YASINSYY, "Comparison of Alternating Direction Time-Differencing Matrods with Other Implicit Mathods for the Solution of the Neutron Group-Diffusion Equations," Nucl. Set Eng., 38, 8 (1989).

TABLE I
Compositions

		Atomic	Number Densit	ies (at/cc ×	1024)	
4 17	Core 1	Core 2	Axial Blanket 1	Axial Blanket 2	Radial Blanket	Reflector
			Models 1 and	2ª .		
²³⁹ Pu	0.001086	0.001501				
238U	0.006383	0.005380	0.008013	0.007383	0.014515	
23 _{Na}	0.01041	0.01098	0.00881	0.00950	0.00660	0.00440
⁵⁶ Fe	0.01814	0.01807	0.02444	0.02385	0.01728	0.06912
160	0.01494	0.01376	0.01603	0.01477	0.02903	
			Model 3			1
²³⁹ Pu	0.0009	0.0013	0.0002	0.0001	0.0003b	
238 _U	0.0055	0.0048	0.0070	0.0070	0.0111 ^b	
²³ Na	0.0120	0.0080	0.0100	0.0070	0.0060 ^b	0.0040
⁵⁶ Fe	0.0180	0.0180	0.0240	0.0240	0.0170	0.0690
160	0.0150	0.0140	0.0160	0.0150	0.0290	

TABLE I Compositions

	k _{et}	ff (% Erro	r)	P _{max} (% error)			
Calculation	Model 1	Model 2	Model 3	Model 1	Model 2	Model 3	
2 SF 4 SF	-0.8 -0.2	-0.2	-0.6 	+1.1	+0.1	-0.8	
6 SF	+0.1	+0.3	+0.1	+0.4	-0.6	+0.6	
2-group	+1.2	+1.2	-6.5	-3.4	-1.0	+5.6	
6-group	+0.4	+0.4	-0.9	+0.7	+0.7	+1.0	

Errors in k_{eff} and Maximum Power Peaking

 $\begin{tabular}{ll} \begin{tabular}{ll} \be$

		Br	eeding Rati	.o ^c	Power Fraction (%)				
Calculation	Total	Axial Blanket	Radial Blanket	Core 1	Core 2	Axial Blanket	Radial Blanket	Core 1	Core 2
24-group	1.164	0.305	0.206	0.499	0.154	1.3	1.3	64.6	32.8
2 SF	1.109	0.260	0.190	0.496	0.164	2.6	2.4	62.3	32.7
4 SF	1.131	0.280	0.195	0.498	0.158	1.7	1.6	63.9	32.8
6 SF	1.136	0.287	0.196	0.496	0.156	1.4	1.3	64.3	33.0
2-group	1.118	0.265	0.196	0.495	0.162	3.0	2.7	62.1	32.2
6-group	1.143	0.289	0.199	0.498	0.157	1.4	1.3	64.3	33.0

TAMLE III
Breeding Mario and Power Fraction, Model I

TABLE IV

Breeding Ratio and Power Fraction, Model 2

		Br	eeding Rati	.o ^c	Power Fraction (%)				
Calculation	Total	Axial Blanket	Radial Blanket	Core 1	Core 2	Axial Blanket	Radial Blanket	Core 1	Core 2
24-group	1.025	0.316	0.063	0.493	0.153	1.4	0.6	63.9	34.1
2 SF	0.943	0.263	0.045	0.476	0.159	2.8	0.7	62.5	34.0
6 SF	0.994	0.295	0.058	0.488	0.153	1.5	0.6	64.3	33.6
2-group	0.970	0.273	0.045	0.490	0.162	3.2	0.7	62.5	33.6
6-group	1.014	0.302	0.059	0.496	0.158	1.5	0.6	63.8	34.1

Breeding Ratio and Fower Fraction, Model 2

 $\label{eq:Table V} Table \ V$ Breeding Ratio and Power Fraction, Model 3

		Br	eeding Rati	.o ^c	Power Fraction (%)				
Calculation	Total	Axial Blanket	Radial Blanket	Core 1	Core 2	Axial Blanket	Radial Blanket	Core 1	Core 2
24-group	1.062	0.285	0.227	0.347	0.203	9.1	4.8	42.9	43.2
2 SF	1.027	0.257	0.210	0.344	0.216	9.5	5.6	41.5	43.4
6 SF	1.044	0.274	0.217	0.347	0.206	8.9	4.7	43.0	43.4
2-group	1.024	0.248	0.198	0.350	0.228	8.3	4.5	41.6	45.6
6-group	1.037	0.271	0.213	0.346	0.206	8.8	4.8	43.0	43.5

Table V Breeding Ratio and Power Fraction, Model 3

 $\label{eq:TABLE VI} \mbox{ Computational Times and Iterations}$

	Model	1	Model	2	Model	3
Calculation	No. Iterations	min ^d	No. Iterations	min ^d	No. Iterations	min ^d
24-group	15	10.90	15	11.26	15	8.87
2 SF	15	2.05	17	1.98	15	1.76
6 SF	16	3.10	16	3.23	14	2.48
2-group	15		15	1.39	15	1.23
6-group	15		15	2.53	15	1.99
24-group/2 SF ^e	7	7.05	7	7.24	7	5.90
24-group/6 SF ^e	7	8.10			6	6.03

Computational Times and Iterati

Footnotes for Tables:

^aFor Model 2, the sodium number density was zero for Core 2 and Axial Blanket 2.

^bFor that portion of the radial blanket which extends above the core axially, ²³⁹Pu = 0.0001, ²³⁸U = 0.0112, ²³Na = 0.0070.

 $^{\text{C}}$ The breeding ratio for a region is defined as the ratio of the ^{238}U capture in that region to the ^{239}Pu absorption in the entire reactor. The total breeding ratio then results as a sum of region breeding ratios.

dCentral Processing Unit, IBM-360-50/75.

^eThe fission source from the 2- (or 6) shape SEF calculation was used as an initial guess in the 24-group calculation. The computing time includes the time required for the SEF calculation and the time required for the 24-group calculation.

Prognotes for lables:

Area ibdel 2, the sodium number density was zero for Core 2 and Axial Signifier 2.

From that portion of the radial blander which extends above the core extends, 138pu = 0.0000, 238pu = 0.0012, 23ka = 0.0070.

Offer broading ratio for a region is defined as the ratio of the ²³⁸U capture in that region to the ²³⁸U absorption in the entire reactor.

The total breeding ratio then results as a sum of region breeding ratios.

The final function source from the 2- (or 6) shape til calculation was used as an initial guess in the 24-group calculation. The computing time includes the time required for the SEF calculation and the time required for the SEF calculation and the time required

FIGURE CAPTIONS

- 1. Two-dimensional LMFBR model.
- 2. Power distribution along vertical centerline (left boundary) for Model 3.
- Power distribution along horizontal centerline (lower boundary) for Model 3.

PLEASER CYLLIAMS

- Lebon SETMI Inclananth-out
- 2. Hower distribution along vertical centerline (left lourday) for Model 3,
 - 3. Power distribution along norizontal centerline (lower boundary) for

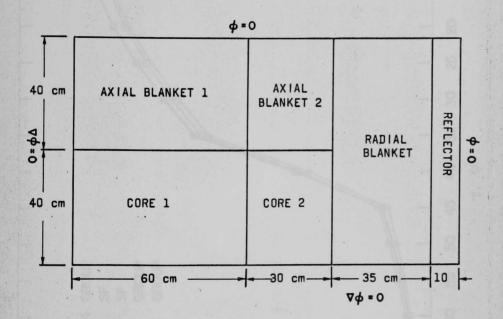


Fig. 1. Two-dimensional LMFBR model.
(ANL Neg. No. 116-634)



Hig. 1, Two-dimensional DMTDR model. (ANL Neg. No. 116-614)

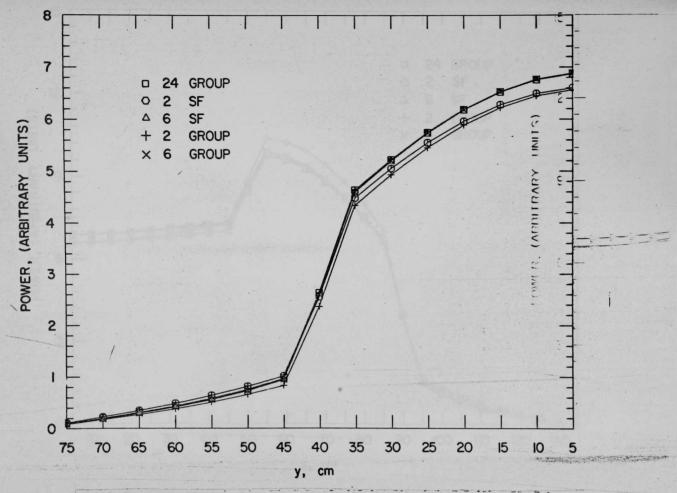
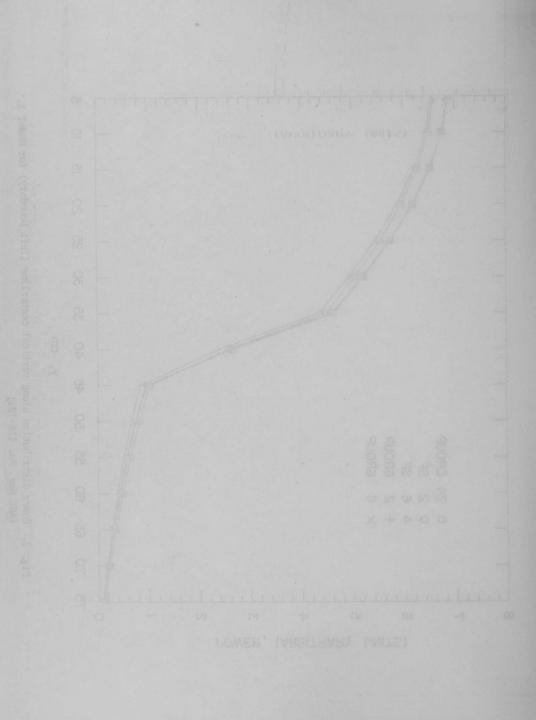


Fig. 2. Power distribution along vertical centerline (left boundary) for Model 3. (ANL Neg. No. 116-701)



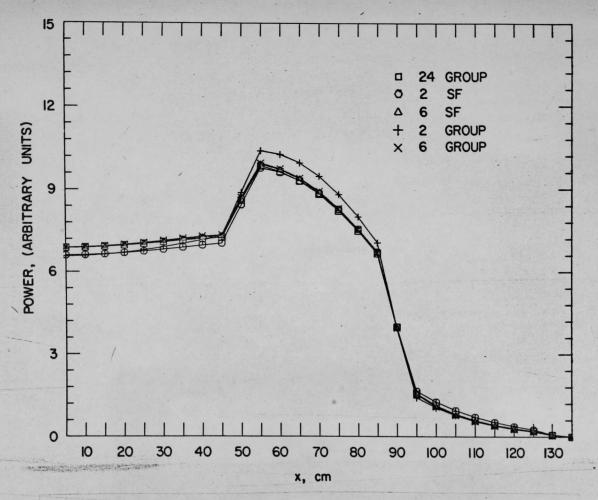


Fig. 3. Power distribution along horizontal centerline (lower boundary) for Model 3.

